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Bulk and surface properties of metal carbides: implications for catalysis

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For this talk, I will describe the results of a comprehensive study into the bulk and surface properties of all available transition metal carbides, with rock-salt structures. I show how the bonding character of these materials is dependent on the periodic position of the transition metal and the direction of the surface termination which in turn tunes the density of states and surface properties.[1] Special consideration is given to the possible implications of these surface properties on the catalysis of CO_2 hydrogenation reactions. The data presented as part of this oral presentation was obtained using Density Functional Theory (DFT) calculation, conducted with the VASP code. A combination of work function and d-band centers provide powerful predictors of catalytic activity towards CO_2 reduction.[2,3]

The development of chemical processes that utilize CO_2 as a heap feedstock, in the production of valuable chemicals, is considered by many as a very important precursor to the future development of a low-carbon economy.[4] Therefore, the primary focus of study is to compare those aspects of transition metal carbides that impact on their future usefulness as catalysts in the conversion of CO_2. To this end, the work that I intend to present at ICCDU XVI severs as a comprehensive screening of the electronic and catalytic properties of many different carbides. The knowledge gained from this study is forming the basis for our current work into the conversion of CO_2 using photo-generated hydrogen.

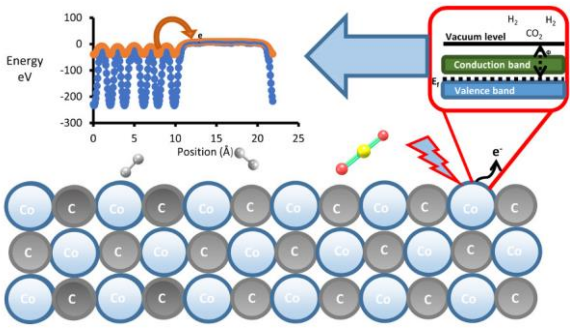

Figure 1. Exploring the implication for CO_2 reduction of a systematic assessment of the carbide surface properties.

Acknowledgments

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References **(Time new roman, 9 pts)**

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